



*Im Rahmen des Physikkolloquiums spricht*

**Dr. Ali Hassanali**

**The Abdus Salam International Centre for  
Theoretical Physics (ICTP) Trieste**

*über*

## **Holes in Liquid Water and Other Hydrophobic Effects**

### **Abstract:**

Density fluctuations in liquid water are at the heart of numerous phenomena associated with hydrophobic effects. One of the most fundamental processes in this regard, is the solvation of hydrophobic solutes in water. The vast majority of theoretical and numerical studies examine density fluctuations at the short length-scale focusing exclusively on spherical cavities. In this work, we use both first principles and classical molecular dynamics simulations to demonstrate that density fluctuations in liquid water can deviate significantly from the canonical spherical shapes. We show that regions of empty space are frequently characterized by exotic, highly asymmetric shapes that can extend far beyond the first solvation shell. Interestingly, density fluctuations of these shapes are characterized by Gaussian statistics with larger fluctuations. An important consequence of this is that the work required to create non spherical cavities can be substantially smaller than that of spheres despite having a much larger surface area. This feature is also qualitatively captured by the Lum-Chandler-Weeks theory. The scaling behavior of the free energy as a function of the volume at short length scales is also qualitatively different for the non-spherical entities. We also demonstrate that non spherical density fluctuations are important for accommodating a hydrophobic amino acid and are thus likely to have significant implications when it comes to solvating highly asymmetrical species such as branched alkanes, polymers or biomolecules.

Time permitting, I will also discuss recent results examining the proton transfer mechanism at the air-water interface and origins of kinetic trapping of protons at the surface of water.

**Datum: Do, 13.10.2016**

**Zeit: 17:15 Uhr**

**Ort: HS 8**